Nuclear Structure and Response based on Correlated Realistic NN Interactions

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Abstract.
Starting from the Argonne V18 nucleon-nucleon interaction and using the Unitary Correlation Operator Method, a correlated interaction v_{UCOM} has been constructed, which is suitable for calculations within restricted Hilbert spaces. In this work we employ the v_{UCOM} in Hartree-Fock, perturbation-theory and RPA calculations and we study the ground-state properties of various closed-shell nuclei, as well as some excited states. The present calculations provide also important feedback for the optimization of the v_{UCOM} and valuable information on its properties. The above scheme offers the prospect of ab initio calculations in nuclei, regardless of their mass number. It can be used in conjunction with other realistic NN interactions as well, and with various many-body methods (Second RPA, QRPA, Shell Model, etc.).

The Unitary Correlation Operator Method (UCOM) provides a novel scheme for carrying out nuclear structure calculations starting from realistic nucleon-nucleon (NN) interactions [1, 2, 3, 4]. The major short-range correlations, induced by the strong repulsive core and the tensor part of the NN potential, are described by a state-independent unitary correlation operator C. This can be used to introduce correlations into an uncorrelated $A-$body state or, alternatively, to perform a similarity tranformation of an operator of interest. Applied to a realistic NN interaction, in particular, the method produces a "correlated" interaction, v_{UCOM}, which can be used as a universal effective interaction, for calculations within simple Hilbert spaces. The same transformation can then be applied to any other operator under study, as is needed for a consistent UCOM treatment.

The utilization of the UCOM involves a cluster expansion of the correlated operators and, currently, a truncation at the two-body (2B) level. The latter is justified by the short range of the correlations treated by the method. The aim is to treat explicitly only the state-independent short-range correlations (SRC); long-range correlations (LRC) should be described by the model space. The correlation functions are determined for each (S,T) channel by minimizing the energy of the two-nucleon system. Three-body interactions are currently not included in the formulation; one way to account for these is by adding a simple phenomenological non-local 2B correction to the correlated Hamiltonian. The introduction of such a correction (the same for all nuclei) has allowed the UCOM to successfully describe properties of nuclei up to mass numbers $A \approx 60$, in the framework of variational calculations within Fermionic Molecular Dynamics [3].

In this work we study nuclear structure and response, based on realistic interactions, without restricting ourselves to light-to-medium systems. This is made possible by employing the v_{UCOM} in Hartree-Fock (HF)- and RPA-based models. The 2B matrix

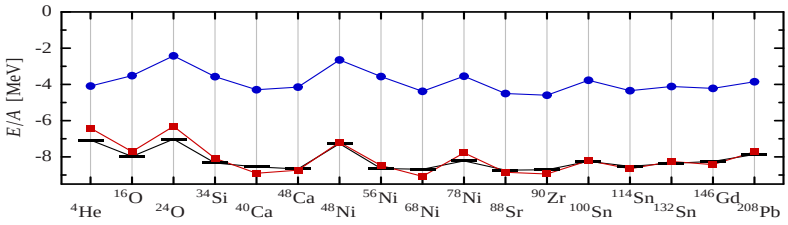

FIGURE 1. Binding energy per nucleon, for the indicated nuclides, in HF (blue dots) and HF+PT (red squares) and experimental (bars).

elements of the v_{UCOM} (without correction terms), Coulomb interaction and (intrinsic) kinetic energy are calculated in a harmonic-oscillator (HO) basis. These are used as input to subsequent HF and RPA calculations, in configuration space. Only spherical, closed-shell nuclei have been considered so far. The following methods have been used:

HF - a spherical-HF method, to estimate at "zeroth order" the nuclear ground state (gs) properties. The HF single-particle states are expanded in the HO basis.

HF+PT - second order perturbation theory (PT) is performed on the HF basis to obtain a correction to the gs energy.

HF+RPA - a self-consistent model, which allows us to estimate a correction to the gs energy due to LRC, and in addition to study collective excitations.

ERPA - an extended RPA [5], which is built on top of the true RPA gs and involves an iterative solution of the RPA equations. Corrected single-particle energies and occupation numbers can be obtained, as well as excitation properties.

The PT and (E)RPA allow us to account for LRC, in addition to the SRC introduced via the UCOM. The optimal separation of the two types of correlations remains an important task. It is expressed primarily by a constraint on the range of the tensor correlation functions, imposed during their parameterization. By varying this range (more precisely, the "correlation volume" I_ϑ [4]), a family of correlators and respective correlated interactions are obtained. Our present results provide important feedback for the optimization of the v_{UCOM} and valuable information on its properties.

The maximum HO-energy and angular-momentum quantum numbers used here are $N_{\max} = 2n + \ell = 12$ and $\ell_{\max} = 10$, respectively, providing a satisfactory degree of convergence. We use the v_{UCOM} parameterizations discussed in Ref. [4], based on the Argonne V18 interaction. The results presented in Figs. 1 and 2 were obtained with $I_\vartheta^{(S=1,T=0)} = 0.09$ fm^3. This value best reproduces, in exact no-core shell model calculations, the binding energy of the light systems ^{4}He, ^{3}H [4].

Ground state properties. Binding is achieved already at the HF level. The inclusion of LRC corrections to the gs energy via PT brings the gs energy very close to the experimental data, as shown in Fig. 1. The RPA correlations result in overbinding [6], mainly due to the double-counting of second-order corrections inherent in the model. In general, larger-I_ϑ tensor correlators provide stronger binding both at the HF and the RPA level. The HF single-particle levels (not shown) are too sparse [6]. The omission of

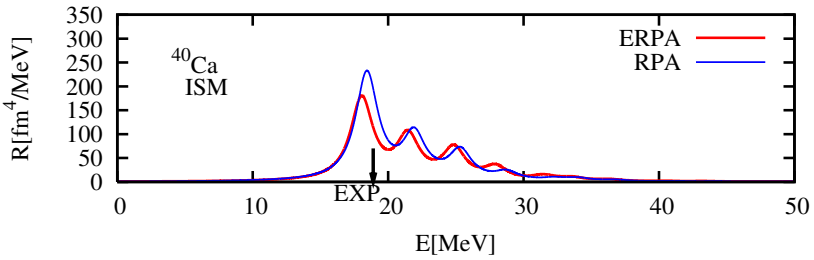

FIGURE 2. Isoscalar monopole resonance of ^{40}Ca, in HF+RPA (blue lines) and ERPA (red lines). An arrow indicates the experimental centroid.

a three-body interaction and of LRC are responsible for this effect. Occupation numbers $n_i = \langle a_i^\dagger a_i \rangle$ (in standard notation) have been calculated within ERPA for ^{16}O and ^{40}Ca. In principle, correlated operators $C^\dagger a_i^\dagger a_i C$ should be used. The small depletion of the Fermi sea that we obtain using uncorrelated operators reflects the effect of the gs LRC [7].

Collective excitations. Our RPA results on the isoscalar (IS) giant monopole resonance (ISGMR), for various medium and heavy nuclei, are in good agreement with the experimental data. An example is shown in Fig. 2, where we see also that the gs correlations taken into account in ERPA have a relatively small effect. In general, lower I_ϑ values result in lower ISGMR energies [6]. The isovector (IV) dipole strength (not shown) is distributed at energies which are too high compared with experiment; ERPA is not able to correct for this result. Inclusion of $2p2h$ configurations within Second RPA is expected to bring the IVD strength to lower energies.

In conclusion, the performance of the v_{UCOM} is very encouraging. Certain aspects of the model (e.g., optimal tensor correlators, three-body effects) are still open to improvement. The above scheme can be used in conjunction with other realistic (local or non-local) NN interactions, as well as with various many-body methods (Second RPA, QRPA, Shell Model, etc), and offers the prospect of ab initio calculations across the nuclear chart.

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